Changes in Ismeans, Version 2.00

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1 Introduction

Versions of Ismeans up through version 1.10 were based on a lot of "spaghetti code" that worked but was increasingly difficult to maintain. So starting with version 2.00, the package underwent a complete overhaul where the code is much more modular and extensible. These changes help make the package better prepared for future use.

Past users of Ismeans may use it in much the same ways as in the old version, but not entirely. And of course, that's the catch—especially when it comes to doing something later with an object created by the lsmeans function. The purpose of this document is to explain the changes that are being made before the package is released, so that users may be prepared for it.

1.1 Availability of old functionality

For a while, the Ismeans package will include a function .old.lsmeans which is the old version of lsmeans from version 1.10-4. Users should adapt to the new lsmeans function as quickly as possible. However, in a clutch, this old one may be used. We use it several tuimes in this diocument to illustrate the differences.

2 Changes that could break existing code that uses Ismeans

2.1 In a nutshell

If you have existing code that extracts or manipulates the result of lsmeans in its old manifestation (i.e. treats it as a list of data.framess); or uses the arguments cov.reduce, fac.reduce, conf, glhargs, lf, or mlf, your code will break as-is. Details follow.

2.2 Returned objects

Probably the most problematic change for past users is that lsmeans used to return a list of data.frames (except sometimes a glht object was thrown in). But now it returns a single object of a new class lsmobj, or a list thereof.

```
R> library(lsmeans)
R> ### OLD
R> warp.lm <- lm(breaks ~ wool * tension, data = warpbreaks)
R> warp.oldlsm <- .old.lsmeans(warp.lm, ~ tension | wool)
R> class(warp.oldlsm)
[1] "lsm" "list"
R> class(warp.oldlsm[[1]])
[1] "data.frame.lsm" "data.frame"
```

```
R> ### NEW
R> warp.lsmobj <- lsmeans(warp.lm, ~ tension | wool)</pre>
R> class(warp.lsmobj)
[1] "lsmobj"
Look at the results obtained the new way:
R> warp.lsmobj
wool = A:
                         SE df lower.CL upper.CL
tension
           lsmean
         44.55556 3.646761 48 37.22325 51.88786
Μ
         24.00000 3.646761 48 16.66769 31.33231
         24.55556 3.646761 48 17.22325 31.88786
wool = B:
                         SE df lower.CL upper.CL
tension
           lsmean
         28.22222 3.646761 48 20.88992 35.55453
         28.77778 3.646761 48 21.44547 36.11008
         18.77778 3.646761 48 11.44547 26.11008
Confidence level used: 0.95
Unlike the old display (not shown), this one pays attention to the | wool part of the specification.
   In the old version, users could access/manipulate the results by taking advantage of the fact that they
inherited from data.frame:
R> ### OLD
R> warp.oldlsm[[1]]$lsmean
[1] 44.55556 24.00000 24.55556 28.22222 28.77778 18.77778
R> Try <- function(expr) tryCatch(expr, error = function(e) cat("Oops!\n"))
R> ### NEW
R> Try(warp.lsmobj$lsmean)
Oops!
The show method for an lsmobj is summary, which indeed does produce an object that inherits from
data.frame. So if you need to access values that you see, call summary first:
R> ### NEW
R> summary(warp.lsmobj)$lsmean
[1] 44.55556 24.00000 24.55556 28.22222 28.77778 18.77778
In casting to data.frame, note that the "by" variable (wool in this case) is included:
R> as.data.frame(summary(warp.lsmobj))
  tension wool
                                SE df lower.CL upper.CL
                  lsmean
```

```
tension wool lsmean SE df lower.CL upper.CL

1 L A 44.55556 3.646761 48 37.22325 51.88786

2 M A 24.00000 3.646761 48 16.66769 31.33231

3 H A 24.55556 3.646761 48 17.22325 31.88786

4 L B 28.22222 3.646761 48 20.88992 35.55453

5 M B 28.77778 3.646761 48 21.44547 36.11008

6 H B 18.77778 3.646761 48 11.44547 26.11008
```

If there is also a contrast specification, then lsmeans does return a list (and not an extension thereof). But each element is of class lsmobj, not data.frame.

```
R> ### NEW
R> warp.12 <- lsmeans(warp.lm, pairwise ~ tension)
R> class(warp.12)
[1] "lsm.list" "list"
R> sapply(warp.12, class)
   lsmeans contrasts
   "lsmobj" "lsmobj"
```

2.3 Changes to cov.reduce and fac.reduce

The cov.reduce and fac.reduce arguments to lsmeans required a second argument giving the name of the variable. This is awkward and, in the case of fac.reduce, doesn't even make sense if you think about it. But if you have existing code that uses these functions, you will have to change it.

In the new version, cov.reduce may be a function or a named list of functions of a single numeric variable. The default is mean. If it is a named list, then a covariate matching a name on the list is reduced using that function, and any mismatched covariates are reduced using mean. As before, cov.reduce may also be logical: TRUE is equivalent to mean, and FALSE is equivalent to function(x) sort(unique(x)).

fac.reduce must now be a function of one matrix argument. Its default is function(X) apply(X, 2, mean). To override it (at least sensibly), you must provide a function that reduces the rows of the matrix into a single vector of the same length.

2.4 Arguments no longer provided

The lsmeans arguments conf, glhargs, lf, and mlf are no longer supported. The needs they serve are supported via lsmobj methods or slots.

Continuing with the warp.lm example and the returned object warp.lsmobj, the conf functionality is replaced by the confint method:

```
R> confint(warp.lsmobj, level = .90)
```

```
wool = A:
 tension
                        SE df lower.CL upper.CL
           lsmean
L
         44.55556 3.646761 48 38.43912 50.67199
М
         24.00000 3.646761 48 17.88356 30.11644
 Η
         24.55556 3.646761 48 18.43912 30.67199
wool = B:
 tension
                        SE df lower.CL upper.CL
           lsmean
L
         28.22222 3.646761 48 22.10579 34.33866
         28.77778 3.646761 48 22.66134 34.89421
M
Η
         18.77778 3.646761 48 12.66134 24.89421
```

The glhargs capability is replaced by an as.glht method to create a glht for use with the multcomp package:

```
R> library(multcomp)
R> summary(as.glht(warp.lsmobj))
```

Confidence level used: 0.9

```
\ast`wool = A`
```

Simultaneous Tests for General Linear Hypotheses

Linear Hypotheses:

```
Estimate Std. Error t value Pr(>|t|)
L, 9 == 0 44.556 3.647 12.218 <1e-07
M, 9 == 0 24.000 3.647 6.581 <1e-07
H, 9 == 0 24.556 3.647 6.734 <1e-07
(Adjusted p values reported -- single-step method)
```

```
\$`wool = B`
```

Simultaneous Tests for General Linear Hypotheses

Linear Hypotheses:

```
Estimate Std. Error t value Pr(>|t|)
L, 9 == 0 28.222 3.647 7.739 < 1e-05
M, 9 == 0 28.778 3.647 7.891 < 1e-05
H, 9 == 0 18.778 3.647 5.149 1.71e-05
(Adjusted p values reported -- single-step method)
```

In lieu of 1f, simply access the linfct slot:

R> warp.lsmobj@linfct

	(Intercept)	woolB	tensionM	tensionH	woolB:tensionM	woolB:tensionH
[1,]	1	0	0	0	0	0
[2,]	1	0	1	0	0	0
[3,]	1	0	0	1	0	0
[4,]	1	1	0	0	0	0
[5,]	1	1	1	0	1	0
[6,]	1	1	0	1	0	1

The mlm argument was new and gave only rudementary support for multivariate responses. Now multivariate predictors cause lsmeans to create one or more additional factors that can be specified in the lsmeans specs. More on this later.

3 Corrections

A few bugs turned up in the course of disciovering that new results did not match old ones—and the new ones were right! Of cours, there could well be undiscovered new bugs.

3.1 Degrees of freedom

Ismeans uses the pbkrtest package to obtain degrees of freedom for models fitted using the Ime4 package. These depend on both the adjusted and unadjusted covariance matrices, but it turns out that the old lsmeans supplied the adjusted one for both. This does not always make a difference:

```
$`Variety lsmeans`
                                      df lower.CL upper.CL
     Variety
                lsmean
                             SE
Golden Rain 105.24081 7.531717 8.458134 88.03504 122.4466
 Marvellous 108.46951 7.482632 8.277316 91.31464 125.6244
     Victory 96.93446 7.641645 8.793756 79.58586 114.2831
$`Variety pairwise differences`
                          estimate
                                         SE
                                                   df t.ratio p.value
Golden Rain - Marvellous -3.228698 6.553848 9.509343 -0.49264 0.87645
Golden Rain - Victory
                          8.306351 6.707936 9.617588 1.23829 0.46004
Marvellous - Victory
                         11.535049 6.670488 9.637889 1.72927 0.24383
    p values are adjusted using the tukey method for 3 means
R> lsmeans(Oats.lmer, pairwise ~ Variety)
$1smeans
Variety
                lsmean
                             SE
                                  df lower.CL upper.CL
Golden Rain 105.24081 7.531717 8.46 88.03704 122.4446
Marvellous 108.46951 7.482632 8.28 91.31571 125.6233
              96.93446 7.641645 8.81 79.59011 114.2788
Results are averaged over the levels of: nitro
Confidence level used: 0.95
$contrasts
 contrast
                           estimate
                                           SE
                                                df t.ratio p.value
Golden Rain - Marvellous -3.228698 6.553848 9.56
                                                   -0.493 0.8764
Golden Rain - Victory
                          8.306351 6.707936 9.80
                                                     1.238 0.4595
Marvellous - Victory
                          11.535049 6.670488 9.80
                                                     1.729 0.2431
Results are averaged over the levels of: nitro
P value adjustment: tukey method for a family of 3 means
The discrepancies are not huge, but they are there. Without the subset that created unbalanced data, the
results essentially agree.
```

3.2 Processing at

In models containing factor or ordered (like Oats.lmer), any at specification was ignored. The new version handles this correctly, including omitting inappropriate levels.

```
R> .old.lsmeans(Oats.lmer, ~ nitro, at = list(nitro = c(.1,.2,.3)))
$`nitro lsmeans`
nitro
         lsmean
                       SE
                                   lower.CL
                                             upper.CL
                                df
   0.0 78.89207 7.294378 7.775291
                                    61.98621 95.79793
  0.2 97.03425 7.136270 7.182133
                                    80.24602 113.82249
   0.4 114.19816 7.136186 7.183591 97.41080 130.98553
   0.6 124.06857 7.070234 6.953145 107.32726 140.80988
R> ### NEW
R> lsmeans(Oats.lmer, ~ nitro, at = list(nitro = c(.1,.2,.3)))
```

```
nitro lsmean SE df lower.CL upper.CL 0.2 97.03425 7.13627 7.19 80.25029 113.8182
```

Results are averaged over the levels of: Variety Confidence level used: 0.95

4 New object structure

The more recent vignettes for Ismeans have explained least-squares means as predictions on a "reference grid," or marginal averages thereof. By default, the reference grid consists of all combinations of factor levels, along with the averages of numeric predictors. But this can be changed by at or cov.reduce. The new design of Ismeans uses a reference-grid object explicitly. For example:

```
R> (Oats.rg <- ref.grid(Oats.lmer))
'ref.grid' object with variables:
    nitro = 0.0, 0.2, 0.4, 0.6
    Variety = Golden Rain, Marvellous, Victory

R> Oats.quad <- update(Oats.lmer, yield ~ Variety + poly(nitro,2) + (1|Block/Variety))
R> ref.grid(Oats.quad)
'ref.grid' object with variables:
    Variety = Golden Rain, Marvellous, Victory
    nitro = 0.31429

R> ref.grid(Oats.quad, at = list(nitro = c(.1,.2,.3)))
'ref.grid' object with variables:
    Variety = Golden Rain, Marvellous, Victory
    nitro = 0.1, 0.2, 0.3
```

The ref.grid function calls two other functions, recover.data (to reproduce the dataset) and lsm.basis (to get the model matrix, coefficients, etc.), each of which has S3 methods for popular model objects like lm, mlm, gls, lmer, etc. This allows ref.grid's capabilities to be easily extended to other model objects not yet supported. ref.grid serves as a constructor for an S4 object of class ref.grid, which encapsulates all the information needed to compute—and make inferences on—least-squares means, independently of the model object itself.

The lsmeans function now consists of S4 methods for a variety of signatures, one of which corresponds to the old version where object is a model object and specs is a formula. So, for example, we may call lsmeans with an existing ref.grid, and provide specifications in place of the old formula interface:

```
R> (Oats.lsm <- lsmeans(Oats.rg, "nitro", by = "Variety"))</pre>
Variety = Golden Rain:
nitro
          lsmean
                       SE
                             df
                                 lower.CL upper.CL
   0.0 80.58462 8.194795 11.70
                                 62.67911
                                           98.49013
   0.2 98.72680 8.020133 10.87
                                 81.04784 116.40577
   0.4 115.89071 8.098890 11.27
                                 98.11673 133.66470
   0.6 125.76112 8.099472 11.21 107.97573 143.54651
Variety = Marvellous:
nitro
          lsmean
                       SE
                             df
                                 lower.CL upper.CL
   0.0 83.81332 8.152095 11.54
                                 65.97327 101.65337
   0.2 101.95550 8.083549 11.19 84.20108 119.70993
   0.4 119.11941 8.005089 10.80 101.45964 136.77918
```

```
Variety = Victory:
nitro
          lsmean
                        SE
                              df
                                  lower.CL
                                            upper.CL
   0.0
        72.27827 8.376203 12.49
                                  54.10747
                                            90.44907
   0.2 90.42045 8.201281 11.58
                                  72.47879 108.36212
   0.4 107.58436 8.200622 11.57
                                  89.64370 125.52503
   0.6 117.45477 8.041801 10.91
                                  99.73629 135.17325
Confidence level used: 0.95
Moreover, lsmobj is in fact an extension of ref.grid, and we can use it as such:
R> str(Oats.lsm)
'lsmobj' object with variables:
    nitro = 0.0, 0.2, 0.4, 0.6
    Variety = Golden Rain, Marvellous, Victory
R> (Oats.n <- lsmeans(Oats.lsm,</pre>
                                 "nitro"))
nitro
          lsmean
                        SE
                             df
                                 lower.CL
                                           upper.CL
   0.0
       78.89207 7.294378 7.78
                                 61.98930
                                           95.79484
   0.2 97.03425 7.136270 7.19
                                 80.25029 113.81822
   0.4 114.19816 7.136186 7.19
                                 97.41454 130.98179
   0.6 124.06857 7.070234 6.95 107.32795 140.80919
```

0.6 128.98982 7.990048 10.71 111.34503 146.63461

Results are averaged over the levels of: Variety Confidence level used: 0.95

4.1 Slots

The classes ref.grid and lsmobj are essentially identical in structure, with lsmobj being a minor extension with the same slots.

R> slotNames(Oats.1sm)

```
[1] "model.info" "roles" "grid" "levels" "matlevs"
[6] "linfct" "bhat" "nbasis" "V" "dffun"
[11] "dfargs" "misc"
```

model.info has the call and terms. roles lists the names of predictors and responses. grid is a data.frame consisting of all combinations of the variables in the list levels. The rows of grid go in one-to-one correspondence with those of linfct, which contains the linear coefficients associated with each LS mean (or reference-grid combination). matlevs has summary information for any matrices in the dataset. bhat holds the regression coefficients. nbasis holds information for determining non-estimability in rank-deficient situations. V is the covariance matrix for bhat. ddfm is a function to return the degrees of freedom for a linear function of bhat. It is passed the contents of the list misc, thus allowing for additional parameters. misc also is used for bookkeeping tasks such as remembering by variables, labels, adjust settings, etc.

5 New functions and methods

There are numerous methods for lsmobj objects. The summary method produces what you see in a listing, and is an extension of data.frame but it is printed with different formatting and with added messages about adjustments, confidence levels, etc. You can also display the results differently. For example:

```
R> summary(Oats.lsm, by = "nitro")
```

(results not shown) will group the Variety means for each nitro rather than the way it is displayed above. There is also and infer argument for flagging whether confidence intervals and/or tests are displayed:

R> summary(Oats.n, infer = c(TRUE,TRUE))

```
nitro
                               lower.CL
                                        upper.CL t.ratio p.value
  0.0
      78.89207 7.294378 7.78
                               61.98930
                                        95.79484
                                                  10.815 <.0001
  0.2 97.03425 7.136270 7.19
                               80.25029 113.81822
                                                   13.597
                                                          <.0001
  0.4 114.19816 7.136186 7.19 97.41454 130.98179
                                                   16.003 <.0001
  0.6 124.06857 7.070234 6.95 107.32795 140.80919
                                                  17.548 < .0001
```

Results are averaged over the levels of: Variety Confidence level used: 0.95

Most other methods are S3 ones, as those are suitable to our needs and often extend existing S3 methods. The as.glht method is illustrated earlier in this document. The confint and test methods are really courtesy methods for summary with argument infer set to c(TRUE, FALSE) and c(FALSE, TRUE) respectively. An important method is contrast:

```
R> (warp.con <- contrast(warp.lsmobj, method = "poly"))</pre>
wool = A:
 contrast
             estimate
                            SE df t.ratio p.value
           -20.000000 5.157299 48
                                   -3.878 0.0003
linear
 quadratic 21.111111 8.932705 48
                                    2.363 0.0222
wool = B:
 contrast
             estimate
                            SE df t.ratio p.value
            -9.444444 5.157299 48
                                  -1.831 0.0733
quadratic -10.555556 8.932705 48 -1.182 0.2432
```

These methods all return new objects of class lsmobj. Hence they may be further analyzed or reanalyzed. For example, suppose we now want to compare the two linear and the two quadratic contrasts in the above:

The pairs method is equivalent to contrast with method = "pairwise". Closely related is the new cld method which produces a compact letter display for which pairwise comparisons are nonsignificant:

```
R> cld(Oats.n, sort = FALSE)
```

```
        nitro
        lsmean
        SE
        df
        lower.CL
        upper.CL
        .group

        0.0
        78.89207
        7.294378
        7.78
        61.98930
        95.79484
        1

        0.2
        97.03425
        7.136270
        7.19
        80.25029
        113.81822
        2

        0.4
        114.19816
        7.136186
        7.19
        97.41454
        130.98179
        3

        0.6
        124.06857
        7.070234
        6.95
        107.32795
        140.80919
        3
```

```
Results are averaged over the levels of: Variety
Confidence level used: 0.95
P value adjustment: tukey method for a family of 4 means
significance level used: alpha = 0.05
```

Finally, there is the lstrends function for estimating fitted trends of a covariate that interacts with a factor. Like the other methods, it returns an lsmobj object, subject to further analysis. To illustrate, the R-provided dataset ChickWeight has data on growth of chicks given different diets. We will fit a random-slopes model and compare the mean slope for each diet. In addition, we'll chose symbols for the display that mimic the grouping lines that some people use.

```
R> chick.lmer <- lmer(weight ~ Time * Diet + (0 + Time | Chick), data = ChickWeight)
R> chick.lst <- lstrends(chick.lmer, ~ Diet, var = "Time")</pre>
R> cld(chick.lst, Letters = "||||")
Diet Time.trend
                        SE
                              df lower.CL upper.CL .group
        6.338556 0.6104878 49.86 5.112266 7.564845
 2
        8.609136 0.8380027 48.28 6.924473 10.293800
                                                     - 11
 4
        9.555825 0.8392450 48.56 7.868917 11.242734
 3
       11.422871 0.8380027 48.28 9.738208 13.107534
                                                       Confidence level used: 0.95
P value adjustment: tukey method for a family of 4 means
significance level used: alpha = 0.05
```

Chicks fed with Diet 3 seem to grow faster than chicks with the other diets, and Diet 1 is the worst.

lstrends uses a difference quotient to do its work, and there is an optional argument delta that can be used to change its increment. It requires a model object—there is no ref.grid method for it. The var argument may imply a function call, i.e. var=sqrt(Time), in which case the chain rule is applied.

6 Support for multivariate models

Ismeans now provides for models with multivariate responses, by way of defining factor levels that index the responses. Thus, linear functions of the multivariate response are available for inference. As an example, consider the package-provided dataset MOats, which is the same as Oats except that each observation is a whole plot with the yields for the four nitro levels as responses.

R> head(MOats)

	Variety	${\tt Block}$	yield.0	<pre>yield.0.2</pre>	yield.0.4	yield.0.6
1	Victory	I	111	130	157	174
2	Golden Rain	I	117	114	161	141
3	Marvellous	I	105	140	118	156
4	Victory	II	61	91	97	100
5	Golden Rain	II	70	108	126	149
6	Marvellous	II	96	124	121	144

Let's fit a model and obtain the reference grid:

```
R> MOats.mlm <- lm(yield ~ Block + Variety, data = MOats)
R> (MOats.rg <- ref.grid(MOats.mlm, mult.levs = list(nitro = c(0,.2,.4,.6))))
'ref.grid' object with variables:
    Block = VI, V, III, IV, II, I
    Variety = Golden Rain, Marvellous, Victory
    nitro = multivariate response levels: 0.0, 0.2, 0.4, 0.6</pre>
```

(The mult.levs argument gives a name and levels for later use; if it had been absent, the multivariate response would have been named rep.meas, with levels 1,2,3,4.)

We may now use nitro just like we would in the univariate case:

```
R> lsmeans(MOats.rg, ~ nitro)
nitro
          lsmean
                       SE df lower.CL upper.CL
   0.0 79.38889 3.198862 10 72.26138 86.5164
  0.2 98.88889 3.811694 10 90.39591 107.3819
  0.4 114.22222 5.020268 10 103.03637 125.4081
  0.6 123.38889 4.216517 10 113.99390 132.7839
Results are averaged over the levels of: Block, Variety
Confidence level used: 0.95
R> lsmeans(MOats.rg, ~ Variety)
Variety
               lsmean
                            SE df lower.CL upper.CL
Golden Rain 104.5000 5.005541 10 93.34696 115.6530
Marvellous 109.7917 5.005541 10 98.63863 120.9447
              97.6250 5.005541 10 86.47196 108.7780
Results are averaged over the levels of: Block, nitro
Confidence level used: 0.95
We can verify that the latter is exactly the same as if we had averaged the responses:
R> MOats <- transform(MOats, avg.yield = apply(yield, 1, mean))</pre>
R> lsmeans(lm(avg.yield ~ Block + Variety, data = MOats), ~ Variety)
                            SE df lower.CL upper.CL
Variety
               lsmean
Golden Rain 104.5000 5.005541 10 93.34696 115.6530
Marvellous 109.7917 5.005541 10 98.63863 120.9447
              97.6250 5.005541 10 86.47196 108.7780
Results are averaged over the levels of: Block
Confidence level used: 0.95
```

7 Support for more models

Several more model types are supported, including survreg, coxph, coxme, and polr models. Here's an example for a Cox proportional-hazards model for the cgd dataset in the survival package:

```
rIFN-g -0.2210687 0.3808731 NA -0.9676565 0.5255192
```

Results are averaged over the levels of: sex Confidence level used: 0.95

8 Transformations

Ismeans tries to discover response transformations and link functions, and provides a type argument in summary, 1smip, and predict that allows inverting the transformation. For example, consider the Cox model just fitted.

```
R> summary(cgd.lsm, type = "response")
inherit = X-linked:
treat
            hazard
                           SE df asymp.LCL asymp.UCL
placebo 1.1328638 0.4196359 NA 0.5480713 2.3416302
rIFN-g 0.3304159 0.1280065 NA 0.1546169 0.7060979
inherit = autosomal:
treat
            hazard
                          SE df asymp.LCL asymp.UCL
placebo 1.8007736 0.4422279 NA 1.1127527 2.9142017
rIFN-g 0.8016616 0.3053313 NA 0.3799725 1.6913367
Results are averaged over the levels of: sex
Confidence level used: 0.95
As another example, suppose we transform the response in warp.lm:
R> logwarp.rg <- ref.grid(update(warp.lm, log(breaks) ~ .))</pre>
R> summary(logwarp.rg)
wool tension prediction
                                 SE df
                3.717945 0.1246647 48
 Α
      L
В
      L
                3.282378 0.1246647 48
 Α
                3.116750 0.1246647 48
В
      Μ
                3.309327 0.1246647 48
 Α
      Η
                3.117623 0.1246647 48
 В
      Η
                2.904152 0.1246647 48
R> summary(logwarp.rg, type = "response")
wool tension lsresponse
                                SE df
                41.17969 5.133656 48
В
      T.
                26.63906 3.320951 48
 Α
      Μ
                22.57289 2.814043 48
В
      Μ
                27.36669 3.411661 48
 Α
      Η
                22.59260 2.816501 48
В
      Н
                18.24975 2.275101 48
```